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NASA TECH BRIEF

A Computer Program for a Line-By-Line Calculation of Spectra from Diatomic Molecules and Atoms Assuming a Voigt Line Profile

The problem:

The task of computing a reasonably accurate spectrum for a mixture of atoms and diatomic molecules is complicated by the enormously large number of rotational lines forming the spectrum. In addition, several kinds of electronic transitions may be involved, each with its own required set of line strength and wavelength equations. These considerations make it impractical to produce the band spectra from even a simple diatomic transition without the aid of an electronic computer.

The solution:

A computer program for predicting the spectra resulting from electronic transitions of diatomic molecules and atoms in local thermodynamic equilibrium.

How it's done:

The program produces a spectrum by accounting for the contribution of each rotational and atomic line considered. The integrated intensity of each line is distributed in the spectrum by an approximate Voigt profile. The program can produce spectra for optically thin gases or for cases where simultaneous emission and absorption occur. In addition, the program can compute the spectrum resulting from the absorption of incident radiation by a column of cold gas or the high-temperature, self-absorbed emission spectrum from a nonisothermal gas. The computed spectrum can be output directly or combined with a slit function and sensitivity calibration to predict the output of a grating spectrograph or a fixed wavelength radiometer.

Specifically, the program has the capability to include the following features in any computation:

1) Parallel transitions ($\Delta\Lambda = \Lambda' - \Lambda'' = 0$), in which spin splitting and lambda doubling are ignored (ignoring spin splitting and/or lambda doubling means that the total multiplet strength is assumed to reside in a single "effective" line).

2) Perpendicular transitions ($\Delta\Lambda = \pm 1$), in which spin splitting and lambda doubling are ignored.

3) $^2\Sigma \longleftrightarrow {}^2\pi$ transitions, in which lambda doubling is ignored.

4) Atomic lines.

5) Option to terminate rotational-line calculations when the molecule dissociates due to rotation.

6) Option to include the alternation of line intensities for homonuclear molecules.

7) Use of an approximate Voigt profile for the line shape.

8) Radiation energy transport in a nonisothermal gas.

The output options available in the program are: (1) Tabulation of the spontaneous-emission spectrum (i.e., optically thin spectrum) for a 1.0 cm path length, (2) Tabulation of the "true" spectrum, which incorporates spontaneous emission, induced emission, absorption, and externally incident radiation through the equation of radiative transfer, (3) Tabulation of the curve of growth for an arbitrary number of wavelength intervals, (4) Tabulation of the integrated intensity over an arbitrary number of wavelength intervals and (5) Tabulation of the output signal produced by a radiometer or spectrometer by specifying an instrument calibration. The instrument slit function can be approximated by up to 99 straight-line segments or by a Gaussian curve. The computation can be made at a fixed wavelength to simulate a radiometer or by

(continued overleaf)

scanning across any specified wavelength interval to simulate a grating instrument. In the latter case, the sensitivity can be varied as a function of wavelength to accurately simulate a grating-instrument calibration.

Notes:

1. This program should be of interest to personnel in the field of quantitative spectroscopy. The program predicts the spectra resulting from electronic transitions of diatomic molecules and atoms in local thermodynamic equilibrium.
2. This program is written in FORTRAN IV for use on the IBM 7040/7094 DCS.
3. Inquiries should be made to:

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   Computer Center
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   Reference: B69-10232

Patent status:

No patent action is contemplated by NASA.

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